*International Journal of*
**QUANTUM CHEMISTRY**

## Contents for Volume XXXVIII, 1990, Nos. 1–6

*Issue No. 1, July 1990*

Non-Radiative Deactivation of Molecules. II. Theoretical Study of the Internal Conversion Rates in Azulene
*K. Gustav and M. Storch* ..... 1

Electrostatic Potential Mapping of Polycyclic Aromatic Hydrocarbon Diol Epoxides Using A Dipole
*A. Kumar and P.C. Mishra* ..... 11

Vibronic Spectral Behavior of Molecules. XIII. Theoretical Contribution to the Vibronic Coupling and the Dushinsky Effect on the $S_1 \leftarrow S_0$ Absorption and the $S_1 \rightarrow S_0$, $S_2 \rightarrow S_1$, and $S_2 \rightarrow S_0$ Fluorescences of Azulene
*K. Gustav and M. Storch* ..... 25

The Symmetrized Basis Function Method for $SU(2)$ and Its Application to the Total Spin States of Many-Electron Systems
*P. Ding, Y. Wang, and Y. Mu* ..... 41

Extrapolation of Finite Cluster and Crystal-Orbital Calculations on *Trans*-Polyacetylene
*E. J. Weniger and C.-M. Liegener* ..... 55

The TST–CEQ Calculations on the Heavy-Light-Heavy CI + CHl Reaction
*G.-Z. Ju and D.-Z. Chen* ..... 75

Theoretical Investigation of the Hydration Properties for the *trans* and *gauche* Rotamers of Succinonitrile
*G. A. Walker, S.C. Bhatia, and J.H. Hall, Jr* ..... 85

**Book Review**

Modelling of Structure and Properties of Molecules.
Edited by Z. B. Maksic
*Reviewed by J.-L. Calais* ..... 93

*International Journal of*
**QUANTUM CHEMISTRY**

## Contents for Volume XXXVIII, 1990, Nos. 1–6

*Issue No. 1, July 1990*

Non-Radiative Deactivation of Molecules. II. Theoretical Study of the Internal Conversion Rates in Azulene
*K. Gustav and M. Storch* ..... 1

Electrostatic Potential Mapping of Polycyclic Aromatic Hydrocarbon Diol Epoxides Using A Dipole
*A. Kumar and P.C. Mishra* ..... 11

Vibronic Spectral Behavior of Molecules. XIII. Theoretical Contribution to the Vibronic Coupling and the Dushinsky Effect on the $S_1 \leftarrow S_0$ Absorption and the $S_1 \rightarrow S_0$, $S_2 \rightarrow S_1$, and $S_2 \rightarrow S_0$ Fluorescences of Azulene
*K. Gustav and M. Storch* ..... 25

The Symmetrized Basis Function Method for $SU(2)$ and Its Application to the Total Spin States of Many-Electron Systems
*P. Ding, Y. Wang, and Y. Mu* ..... 41

Extrapolation of Finite Cluster and Crystal-Orbital Calculations on *Trans*-Polyacetylene
*E. J. Weniger and C.-M. Liegener* ..... 55

The TST–CEQ Calculations on the Heavy-Light-Heavy CI + CHl Reaction
*G.-Z. Ju and D.-Z. Chen* ..... 75

Theoretical Investigation of the Hydration Properties for the *trans* and *gauche* Rotamers of Succinonitrile
*G. A. Walker, S.C. Bhatia, and J.H. Hall, Jr* ..... 85

**Book Review**

Modelling of Structure and Properties of Molecules.
Edited by Z. B. Maksic
*Reviewed by J.-L. Calais* ..... 93

*Issue No. 2, August 1990*

Title Page ..... 95

Rudolph Zahradník ..... 97

Publications of Rudolph Zahradník ..... 99

Biographical Information ..... 115

Introductory Remarks ..... 119

Optimum Structures and Vibrational Frequencies of $(SiC)_2$ Clusters
*G. B. Fitzgerald and R. J. Bartlett* ..... 121

Solvent Effects on Mechanism of Tetramethylene Polymerization
*K. Jug* ..... 129

Applications of the MBPT in the Localized Representation
*E. Kapuy, F. Bartha, F. Bogár, Z. Csépes, and C. Kozmutza* ..... 139

Triplet-Singlet Splitting of the Alkali Metal Clusters: Example of the $Li_6$ Clusters
*J. Koutecký, I. Boustani, and V. Bonačić-Koutecký* ..... 149

Computational Chemistry on a PC
*G. Náray-Szabó, J. G. Ángyán, P. R. Surján, Z. Szalóczy, K. Ösapay, I. Kövesdi, and I. Kolossváry* ..... 163

Spectroscopic Studies on the Protonation of Schiff Bases
*R. Bicca de Alencastro, S. Badilescu, L. S. Lussier, C. Sandorfy, H. Le Thanh, and V. Vocelle* ..... 173

Intermolecular Interactions with the Direct Reaction Field Method
*P. Th. van Duijnen and J. A. C. Rullmann* ..... 181

Theoretical Approach to Reactions of Polyatomic Molecules
*L. Zülicke and A. Merkel* ..... 191

Nonlinear Coupling in the Quantum Statistical Theory of Proton Transfer Dynamics
*P. Baňacký and A. Zajac* ..... 209

Localization of Virtual Orbitals
*F. Bartha, F. Bogár, and E. Kapuy* ..... 215

MNDO Calculation of Reaction Heats Determining the Mechanism of Antioxidant Action of the Phenols in Polyolefins
*A. Bolotin and P. Pipiraité* ..... 221

Investigation of the Influence of the Substitutes on the Intensity of the Absorption Band of Some Polymethine Dyes
*L.-M. Balevičius, A. Bolotin, and D. Shatkovskaya* ..... 225

MNDO CI Study of the Photoisomerization About Polar Double Bonds
*P. Ertl* ..... 231

Quantum Chemical Calculations of Silicon Clusters in Silicon Dioxide and Point Defects in β-Cristobalite
*G.V. Gadiyak, I.V. Korolenko, and Yu. N. Morokov* ..... 239

Double Bonds in the Second and Third Periods. Ab Initio Study of the Conjugation in $H_nX{=}YH_m{-}ZH_2$ (X,Y = C, N, Si, and P; Z = B and N; $n = 1, 2$; $m = 0, 1$)
*A. A. Korkin* ..... 245

Graph Theory of Synthons
*V. Kvasnička and J. Pospíchal* ..... 253

Ground-State Multiplicity by Spin-Extended Hartree–Fock Method
*M. M. Mestechkin and G. E. Whyman* ..... 279

Ab Initio Calculations of Nuclear Quadrupole Coupling Constants of Low-lying Rovibrational Levels in the $X^1\Sigma^+$ and $A^1\Sigma^+$ States of All Isotopic Species of LiH
*I. Paidarová, J. Vojtík, L. Češpiva, J. Šavrda, and V. Špirko* ..... 283

Transfer of Electronic Excitation Energy in Partially Disordered Polymer Chain
*T. Pálszegi and O. Kyseľ* ..... 297

Nonstandard Turn of MDGI Protein Binding Site of Fatty Acids?
*R. Suessmilch, J. Jaeger, and J. Behlke* ..... 311

QCT Study of Isotopic Effects in H + HBr Abstraction and Exchange Reactions
*J. Tiňo, J. Urban, and V. Klimo* ..... 321

The Method of Moments and Chemical Bonding: Interaction of Two Adatoms on Simple Cubic and *B.C.C.* Transition Metal (001) Surfaces
*S. Pick, M. Tomášek, and M.U. Luchini* ..... 329

Theoretical Study of the Reaction Ne + $H_2^+ \rightarrow NeH^+ + H$ in the $^2A'$ Ground State
*J. Urban, R. Jaquet, and V. Staemmler* ..... 339

1*s* Core-Level Shifts of Al and Ar Atoms in Aluminum Clusters
*ZS. Varga and I. K. Gyémánt* ..... 351

Theoretical Description of Nuclear Quadrupole Coupling in Light Diatomic Molecules
*J. Vojtík, I. Paidarová, V. Špirko, J. Šavrda, and M. Petráš* ..... 357

Variational Calculations of the Wigner Distribution Function for Selected Anharmonic Oscillators
*J. J. Włodarz and J. Nowakowski* ..... 373

*Issue No. 3, September 1990*

Optimization of Molecular Electronic Structure Calculations. 1. Local Symmetry and Local Symmetricized Orbitals
*A. B. Kovrikov* ..... 383

Optimization of Molecular Electronic Structure Calculations. 2. Calculation of Symmetry-Reduced Matrix Elements
*A. B. Kovrikov* ..... 389

Density Matrix of Crystalline Systems. I. Long-Range Behavior and Related Computational Problems
*C. Pisani, E. Aprà, and M. Causà* ..... 395

Density Matrix of Crystalline Systems. II. The Influence of Structural and Computational Parameters
*C. Pisani, E. Aprà, M. Causà, and R. Orlando* ..... 419

Squeezing Transformation Caused by Frequency Jumps for Solving the Problem of Two Coupled Oscillators
*H.-Y. Fan* ..... 435

Molecular Integrals in the Generalized Hylleraas-CI Method
*Y. Lu and Z. Huang* ..... 447

Sur Une Tentative D'Unification des Théories Quantiques de la Cancérisation par les Polyacènes: I. Théorie des Régions M, L, et B
*J. Gayoso and S. Kimri* ..... 461

Sur Une Tentative D'Unification des Théories Quantiques de la Cancérisation par les Polyacènes. II: Le Rôle de la Region K dans le Processus D'Activation Metabolique Conduisant au Cancérogène Ultime. Théorie des Régions M, L, et BK
*J. Gayoso and S. Kimri* ..... 487

**Book Review**

Theory of Molecular Fluids. Volume 1: Fundamentals. By C. G. Gray and K. E. Gubbins
*Reviewed by J.-L. Calais* ..... 497

**Erratum**

Role of Doubly Excited States in Calculations of Optical Activity
*A. Volosov* ..... 499

*Issue No. 4, October 1990*

Physical Quantification of the Biological Effectiveness of Ionizing Radiations
*D. E. Watt and L. A. Kadiri* ..... 501

Tunnel Effect in Proton Transfer
*J. L. Esquivel and J. F. Mata-Segreda* ..... 521

A Study of Hydration Effects on the Conformational Aspects of GABA Mediators
*D. Majumdar and S. Guha* ..... 533

Splitting of $n$-Fold Rotationally Symmetric Graphs
*M. Shen* ..... 551

Application of Molecular Orbital Graph Theory to Vibrational Problems of Finite Chain Systems
*T. Lü, A. Tachibana, and T. Yamabe* ..... 559

Modeling of Real 20-Component Protein Chains: Determination of the Electronic Density of States of Aperiodic Seven-Component Polypeptide Chains Containing Strongly Different Amino Acid Residues
*A. K. Bakhshi, P. Otto, C.-M. Liegener, and J. Ladik* ..... 573

Electron Correlation Described by Extended Geminal Models: The EXGEM7 and EXRHF3 Models
*I. Røeggen* ..... 585

A Population Analysis Based on Hybrid Orbitals
*L. Ming* ..... 597

**Book Review**

Large Finite Systems. Proceedings of the Twentieth Jerusalem Symposium on Quantum Chemistry and Biochemistry. Edited by J. Jortner, A. Pullman, B. Pullman, and D. Reidel
*Reviewed by J.-L. Calais* ..... 607

Announcement ..... 609

*Issue No. 5, November 1990*

Preface ..... 611

EUCHEM Conference Tromsø, June 20, 1989 ..... 613

Theoretical Study of Single-Electron Capture in the $N^{5+}$ + He and $O^{6}$ + He Collisions by Means of Ab Initio Methods
*M.C. Bacchus-Montabonel and K. Amezian* ..... 615

The Modeling of Nucleophilic and Electrophilic Additions and Substitutions Using Extended Hückel-based Reaction Potentials
*C. Daul, A. Goursot, P.-Y. Morgantini, and J. Weber* ..... 623

Methods for Electron Correlation on Large Molecules
*S. Sæbø* ..... 641

Transition Structures and Energy Barriers of Pericyclic Reactions in the CASSCF Approach
*R. Janoschek and J. Kalcher* ..... 653

Localized Orbitals for the Description of Molecular Interaction
*C. Kozmutza and E. Kapuy* ..... 665

Covalent and Ionic Contributions to the Bonding of Atomic and Molecular Adsorbates on Metal Surfaces: A Cluster Model Approach
*G. Pacchioni, P.S. Bagus, M.R. Philpott, and C.J. Nelin* ..... 675

Density Functional Calculation of Transition Metal Cluster Energy Surfaces
*S. A. Beznosjuk, R. D. Dajanov, and A. T. Kuldjanov* ..... 691

Molecular Point Symmetry and the Phase of the Electronic Wave Function: Tools for the Prediction of Critical Points of Potential Energy Surfaces
*P. G. Mezey* ..... 699

Analysis of Molecular Shape Changes Along Reaction Paths
*G. A. Arteca and P. G. Mezey* ..... 713

Exploring the Potential Energy Hypersurface of Histamine Monocation: Tautomerism in Gas Phase
*O. Tapia, R. Cárdenas, Y. G. Smeyers, A. Hernández-Laguna, J. J. Rández, and F. J. Rández* ..... 727

On the Long Way from the Coulombic Hamiltonian to the Intermolecular Energy Surfaces: Concluding Remarks at the Tromsø Conference June 20–22, 1989
*P.-O. Lowdin* ..... 741

Announcement ..... 759

*Issue 6, December 1990*

Applicability of Multi-Reference Many-Body Perturbation Theory to the Determination of Potential Energy Surfaces: A Model Study
*S. Zarrabian and J. Paldus* ..... 761

Approximating Quasi-Particle Density Functional Calculations of Small Active Clusters: Strong Electron Correlation Effects
*S. A. Beznosjuk, B. F. Minaev, R. D. Dajanov, and Z. M. Muldakhmetov* ..... 779

The Effect of Interlayer Interactions on Chemisorption Pattern Stability: Hydrogen Atoms on Graphite
*J. P. LaFemina* ..... 799

Approximate Density Matrices and Wigner Distribution Functions from Density, Kinetic Energy Density, and Idempotency Constraints
*R. C. Morrison, W. Yang, R. G. Parr, and C. Lee* ..... 819

Explicit Algebraic Form of Coupled Cluster Equations for the PPP Model of Benzene with an Approximate Inclusion of Triexcited Clusters
*J. Čížek, F. Vinette, and J. Paldus*..... 831

The Virial Theorem Scaling Model for Estimating the Charge Sensitivities of Hydrogens in Molecules
*M. Streszewski and R. F. Nalewajski*..... 853

**Book Reviews**

Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules. Edited by M. Defranceschi and J. Delhalle
*Reviewed by J.-L. Calais*..... 865

Hyperspherical Harmonics. Applications in Quantum Theory. By J. Avery
*Reviewed by J.-L. Calais*..... 867

Density Matrices and Density Functionals. Proceedings of the A. John Coleman Symposium. Edited by R. Erdahl and V. H. Smith, Jr.
*Reviewed by J.-L. Calais*..... 869

**Erratum**

Two-center Molecular Repulsion Integrals Over Slater Functions
*E. N. Maslen and M. G. Trefry*..... 871

Author Index to Volume XXXVIII..... 873

Subject Index to Volume XXXVIII ..... 877

Volume Title Page ..... v

Volume Contents ..... vi